MALCOLM PIRNIE

INTEROFFICE CORRESPONDENCE

To: Ed Garvey **Date:** 09/26/2008

Copy: Shane McDonald, Scott Thompson, Bruce Fidler

From: Solomon Gbondo-Tugbawa and Chris Gurr, NNJ

Re: Uncertainty Analysis on the Empirical Mass Balance (EMB) and Forecast Trajectories

Summary

An uncertainty analysis was performed on the EMB and on the forecast trajectories for seven contaminants of concern. The goals of the analysis were two-fold:

- to estimate the range of uncertainty (*i.e.* the confidence levels) for the empirical mass balance conducted for 2007, that is for both the solids balance and the chemical mass balances; and
- to estimate the range of uncertainty for the forecasts of chemical concentrations under MNR, a 30 percent remediation of RM0 to RM8, and a complete remediation of RM0 to RM8.

A Monte Carlo sampling approach was used to develop 10,000 iterations of input parameters for the EMB and for the forecast models. The distribution of model outputs was used to assess variability in model results.

The EMB Monte Carlo simulations of recently deposited solids in the Lower Passaic River indicate that resuspension represented 45 percent on average of recently deposited material, with a 5 to 95 percent confidence interval of 28 to 65 percent. This agrees with the original EMB estimate reported in the Conceptual Site Model (CSM). In the Monte Carlo analyses, Newark Bay accounted for an average of 17 percent, with a range from less than 1 to 44 percent in recently deposited sediment. The original EMB estimate for Newark Bay was 27 percent. Furthermore, the Monte Carlo analysis suggests that the Upper Passaic River accounted for an average of 31 percent, with a range from 13 to 49 percent. The original EMB estimate for Upper Passaic River estimate was 23 percent. The differences in the relative contributions of Newark Bay and the Upper Passaic River between the Monte Carlo results and previous results in the CSM are not attributable to the refinement in the uncertainty analysis but are rather due to the exclusion of a single outlier sample, as described below.

As was observed with the deterministic EMB calculations presented in the CSM, the fate and transport of the chemicals as simulated by the Monte Carlo analysis were dominated by resuspension, with the exception of PAHs. For PAHs, a larger percentage originates from the Upper Passaic River. For 2,3,7,8-TCDD, resuspension accounts for an average of 95 percent of the contaminant burden in recently deposited sediments, with the low end estimate of the resuspension contribution at more than 87 percent.

Uncertainty in trajectory forecasts for contaminant concentrations in the mixed (or active) surface layer included using the uncertainty analysis developed for the EMB combined with additional variability in the distributions developed for the remaining parameters used in the forecast model (*e.g.,* “excess” contaminant half lives, mixed layer thickness, sediment deposition rate). Again a series of 10,000 iterations were run for the forecast of each contaminant, each one corresponding to one of the 10,000 iterations of the EMB. Uncertainty in trajectory forecasts was depicted as confidence bounds associated with predicted future chemical concentrations. In general, the remediation of the primary inventory and erosional zones (30 percent cap scenario) did not result in any sustained benefits compared to monitored natural remediation (MNR). The most significant benefit from remediation results from improvements in 2,3,7,8-TCDD surface sediment concentrations under remediation of RM0 to RM8 scenario. The recovery of the 2,3,7,8-TCDD in surface sediment predicted for the RM0 to RM8 remedial scenario appears to be slightly enhanced in the uncertainty analysis, which is attributed to the reduction in the Newark Bay contribution. This analysis does not incorporate any further recovery enhancement by continued channel dredging in Newark Bay, which should accelerate the reduction in the input concentrations from this end member. Because the concentrations in the external sources for the other parameters forecasted are significant, the overlap in the predicted sediment concentrations for these compounds based on the RM0 to RM8 remedial scenario and the MNR remedial scenario occurs around or before the year 2060.

Objectives of the Analysis

1. To provide insight into the level of confidence in the solids and chemical mass balances constructed as part of the EMB.
2. To incorporate the uncertainties of the EMB analysis as well as other forecast model parameters into an assessment of the forecast uncertainty for seven major contaminants of concern.

Methodology

The input data required for the EMB include the chemical concentrations for the sources (Resuspension, Newark Bay, Upper Passaic River, Tributaries and CSO) and the receptor (Lower Passaic River; RM2 to RM12). Uncertainties in these inputs were simulated by a Monte Carlo[1] sampling approach to develop 10,000 iterations of each input as follows:

- For external sources and receptor, a bounded normal distribution defined by the mean, standard deviation, minimum and maximum observed concentration of each chemical was used to perform Monte Carlo simulation. The results of simulation are shown in Figures 1a-g. A total of 12 compounds were incorporated

[1] Monte Carlo simulation is a statistical sampling method in which the trails or realizations (*i.e.*, individual values) are randomly generated from probability distributions to simulate the process of sampling from an actual population.

in the analysis in this fashion. Total organic carbon was also sampled in this manner but was not included directly in the optimization.

- For resuspension, a bootstrap[2] approach was used to simulate the 10,000 iteration since the 1995 TSI data was neither normal nor log-normal and thus could not be approximated like the external sources. TSI location 246 was excluded because it was determined to be an outlier for PAHs (Figure 1h).
- The correlations among the chemicals for each source and receptor were maintained by randomly selecting the samples themselves, (and not the individual contaminant concentrations) to ensure that the 10,000 iterations of chemical profiles represented the chemical inter-dependencies.

For the COPC forecast calculations, the inputs include: the chemical concentrations inputted into the EMB uncertainty analysis, the EMB uncertainty analysis output for solids balance, the decay of excess sediment contaminant concentrations (lambda; λ, from the dated sediment cores corrected for baseline levels), the net sedimentation rate, and depth of sediment mixed layer. Uncertainties in these inputs were defined as follows:

- Uncertainties in the chemical concentrations to the EMB are described above (Figure 1).

- Uncertainties in solids contribution from the various sources were obtained from the uncertainty in the solids contributions determined by the EMB uncertainty analysis.

- Uncertainties in decay of excess sediment contamination were defined by the regression between the natural logarithm of the excess concentrations versus time (Figure 2). This was estimated from the 5 dated sediment cores, similar in fashion to the original forecast analysis. Using the slope (λ), standard error and confidence bounds from the regressions, 10,000 iterations of λ were simulated using Monte Carlo sampling from bounded normal distributions (Figure 3). With the exception of chlordane, the λs for the other chemicals are statistically significant. Note the half life is related to λ as follows: $Half\ life = \ln(0.5)/\lambda$

- Uncertainties in the sedimentations rates were generated by bootstrap analysis of the differences between the 1989 and 2007 bathymetric surfaces (Figure 4).

- Uncertainties in the estimate of the depth of sediment mixed layer were generated by 10,000 random numbers between 10 cm to 20 cm in Excel (Figure 5).

[2] Bootstrap is a powerful Monte Carlo method that re-samples the original sample set with replacement to generate a distribution of sample's statistics. It is a non-parametric method.

Previous Excel spreadsheets designed for EMB and forecast calculations were used for this analysis. To automate the process of performing 10,000 calculations, Excel macros[3] were written to: read the inputs into the spreadsheets, call applicable functions, and save the outputs.

EMB Results

The analysis of uncertainty for the EMB is summarized in Table 1 and described below. In each description, the range represents the 5th and 95th confidence limits for the source contribution:

- Of the total solids recently deposited in the Lower Passaic, solids balance results (Figure 6) indicate:
    - Resuspension accounted for an average of 45 percent of the solids in recently deposited sediments, with a range from 28 to 65 percent.
    - The Upper Passaic River accounted for an average of 31 percent with a range from 13 to 49 percent.
    - Newark Bay accounted for an average of 17 percent with a range from less than 1 to 44 percent.
    - All the other solids sources together contribute between 2 and 12 percent with an average of 7 percent.
- Fate and Transport plots indicate (Figures 6 to 19) that resuspension is the dominant flux for all chemicals simulated except for PAHs, for which the Upper Passaic River is the largest single contributor. For dioxins, ~ 87 percent or more of the burden in recently deposited sediments originates from resuspension. Note that the Lower Passaic River concentration in the plots is the receptor concentration for the EMB.
- Table 1 compares average results from the 10,000 simulation to results previously reported as part of the deterministic analysis in the CSM. While solids contribution from resuspension remained unchanged, this analysis indicates fewer solids from Newark Bay and more solids from the Upper Passaic River. The reason for these differences is because the PAH outlier at TSI location 246 was included in the deterministic analysis reported in the CSM and not included in this analysis. This difference in solids balance also resulted in generally minor changes in the relative chemical fluxes to the Lower Passaic River (Table 1).

Trajectory Forecast Results

Figures 20 to 26 present the uncertainty bounds on the COPC forecasts defined by the 5th and 95th percentiles of the simulated results. The results can be summarized as follows:

- The remediation of primary erosional and inventory zones (30 percent cap scenario) will not result in sustained benefit relative to MNR.

[3] An Excel macro is a set of instructions written in Visual Basic programming language for Application that can be triggered by a keyboard shortcut, toolbar button or an icon in a spreadsheet. Macros are used to eliminate the need to repeat the steps of common tasks over and over.

- For dioxin, a significant improvement in surface sediment concentrations results from RM0 to RM8 Cap scenario. The upper confidence bound for this scenario does not intersect the lower confidence bound for MNR until 2083, more than 60 years beyond implementation of the remedy.
- For all the other COPC forecasted (mercury, TPCB, copper, 4,4'-DDE, lead) the importance of external sources impact their recovery and future concentrations, despite the importance of resuspension to their current loads. This is a direct result of relatively high concentrations of these compounds in the external solids sources. The importance of the resuspension mechanism to their current (2007) mass balance reflects the large magnitude of this solids source rather than the presence of notably higher concentrations, unlike the 2,3,7,8-TCDD mass balance.
- As shown in Figure 3b, the half lives of the excess concentration for most contaminants overlaps in the range of 23 to 33 years, with several centered in this range. This observation suggests that a single mechanism, *i.e.*, the resuspension process and the associated mass of legacy sediment is likely responsible for this gradual decline, buffering the "excess" contamination levels for each of these contaminants.